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S. A. Berestova, N. P. Kopytov, N. E. Misura, and E. A. Mityushov

Texture Parameter Variation Region for Orthotropic Polycrystals with Cubic Symmetry of the Crystal Lattice

S. A. Berestova[a)], N. P. Kopytov[b)], N. E. Misura[c)], and E. A. Mityushov[d)]

Ural Federal University named after the First President of Russia B.N. Yeltsin,
19 Mira St., Ekaterinburg, 620002, Russia

[a)]Corresponding author: s.a.berestova@urfu.ru
[b)]nikitako@mail.ru
[c)]n_misura@mail.ru
[d)]mityushov-e@mail.ru

Abstract. The variation region of texture parameters (which are integral characteristics of the preferable orientation of crystallographic axes) allows solutions to be found for managing anisotropic properties, illustrating all possible textured states of an orthotropic polycrystalline material with a crystal lattice of cubic symmetry. Each point in this region is matched by certain anisotropy of both elastic and plastic properties. The region of texture parameter variation is defined both analytically and using a numerical experiment of statistic simulation. Analytically, the solution is found via determining the effective eigenvalues of the elasticity operator for a textured anisotropic cubic polycrystal. The algorithm to be followed for visualizing the region-forming elements implies determining the lines of intersection of planes with a conical surface. The numerical solution is based on the determination of texture parameters, i.e, on the starting assumption that the variation region is bounded and lies in the first octant. The task of constructing the variation region is solved via finding the texture parameters using the Monte-Carlo method according to the density of distribution of crystallographic axes in space. When modeling the variation region, octets are used, which are symmetrical reflections of randomly taken orientations in all the octants of space. The constructed regions have the required symmetry. The numerically obtained cloud of textured states and the analytically constructed variation region have geometric centers coinciding at the point corresponding to the non-textured state. At various stages of thermal and mechanical treatment of metallic materials, texture evolution can be represented geometrically as a texture state trajectory that is seen to be within the determined texture parameter variation region..

TEXTURE PARAMETERS OF ANISOTROPIC POLYCRYSTALS

Using mathematical models to relate internal parameters of a material with its texture, i.e., with the preferable orientation of crystallographic axes occurring in the process of plastic deformation, opens up a scientifically grounded opportunity to manage the physical and mechanical properties of a material. For orthotropic textured metals and alloys having a crystal lattice of cubic symmetry, the physical and mechanical properties are determined by structural parameters of stochastically geometric significance, which are defined by the following equations:

$$\Delta_i = \left\langle Q_{i1}^2 Q_{i2}^2 + Q_{i2}^2 Q_{i3}^2 + Q_{i3}^2 Q_{i1}^2 \right\rangle \ (i = 1,2,3)\,,$$

where Q_{ij} are the elements of the matrix of direction cosines, which determine the positions of crystallographic axes for randomly oriented grains of a polycrystal in the laboratory frame of coordinates related to an orthotropic sample, and $\langle ... \rangle$ represents the procedure of averaging over a representative volume of the textured polycrystal.

Texture parameters referred to as orientation factors were first introduced in [1] in order to determine a quantitative relation of the crystallographic texture to the elastic properties of *bcc* and *fcc*-structured polycrystals.

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Later, these parameters were given other names, such as anisotropy invariants, integral characteristics of texture, deformation anisotropy parameters; these names have reflected their mathematical and physical essences [2, 3].

Each texture of an orthotropic material has corresponding values of texture parameters, which may be viewed as a point in the texture parameter space. For a polycrystalline aggregate, a set of textured states is characterized by a certain closed region. Generally speaking, probable anisotropy of an orthotropic textured polycrystal having a cubic symmetry structure is determined with a certain region of texture parameter variation. For a geometric representation of the variation region, the Cartesian coordinate system is used, where along each of the axes there is a value plotted for the corresponding texture parameter.

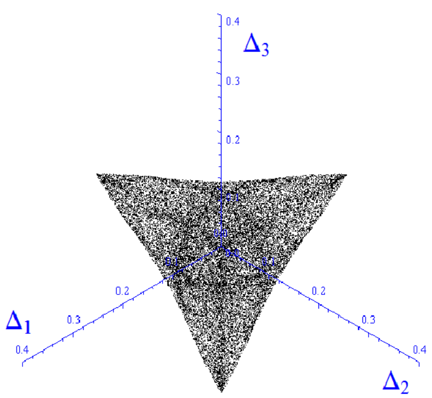
NUMERICAL EXPERIMENT FOR PLOTTING A TEXTURE PARAMETER VARIATION REGION

The variation region of texture parameters can be obtained via numerical experiment. Statistical simulation can be applied for visualizing the region of all possible states of orthotropic polycrystalline material of a cubic structure in the texture parameter space. The numerical solution is based on determining the texture parameters, i.e., it is assumed from the start that the variation region is bounded and lies in the first octant. The problem for constructing the variation region is solved via finding the texture parameters applying the Monte-Carlo method determining the parameters according to the density of crystallographic axes distribution in the space. For variation region simulation, the octets are used which are symmetrical reflections of randomly taken orientations over all the octets in the space. By generating a set of octets of random orientations, the corresponding texture parameters are calculated, i.e. the points are determined in the region displayed in Fig. 1.

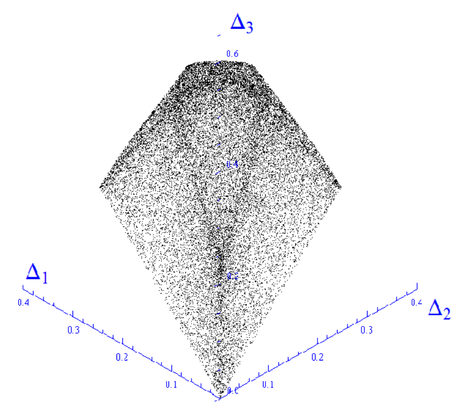
Each random orientation has its corresponding matrix of direction cosines:

$$M(\psi,\theta,\varphi)=\begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}=\begin{pmatrix} \cos\psi\cos\varphi-\sin\psi\cos\theta\sin\varphi & -\cos\psi\sin\varphi-\sin\psi\cos\theta\cos\varphi & \sin\psi\sin\theta \\ \sin\psi\cos\varphi+\cos\psi\cos\theta\sin\varphi & -\sin\psi\sin\varphi+\cos\psi\cos\theta\cos\varphi & -\cos\psi\sin\theta \\ \sin\theta\sin\varphi & \sin\theta\cos\varphi & \cos\theta \end{pmatrix},$$

where ψ, θ, φ are Euler angles.



(a)



(b)

FIGURE 1. Numerically obtained region of possible states of an orthotropic polycrystalline material with a cubic structure. Viewpoints: {3,3,3} (a), {10,10,-10} (b)

Realizing plane symmetrical reflections of this matrix in the sequence

$$\Delta_1 O\Delta_3 \to \Delta_2 O\Delta_3 \to \Delta_1 o\Delta_3 \to \Delta_1 O\Delta_2 \to \Delta_2 O\Delta_3 \to \Delta_1 O\Delta_3 \to \Delta_2 O\Delta_3$$

and using, respectively, the transformation matrices

$$L_{\Delta_1 O \Delta_3} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ L_{\Delta_2 O \Delta_3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ L_{\Delta_1 O \Delta_2} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

the matrixes of direction cosines are obtained for eight orientations to form an octet. The octet has three symmetry planes with respect to the frame of coordinate planes. Considering this octet as a model of "random" orthotropic material, a procedure of calculating the texture parameters is carried out. Orientations of each octet are generated using a simulation function for the distribution of the Euler angles, which corresponds to the non-textured state of a polycrystalline material.

ANALYTICAL METHOD FOR CONSTRUCTING THE VARIATION REGION OF TEXTURE PARAMETERS

Such a region can also be constructed analytically, from the condition of the weighting factors being positive in the corresponding averaging job, to determine the average weighted effective eigenvalues of the elasticity operator for an anisotropic polycrystalline material with a lattice of cubic [4]:

$$\Delta_1 + \Delta_2 + \Delta_3 - 2\sqrt{\Delta_1^2 + \Delta_2^2 + \Delta_3^2 - \Delta_1\Delta_2 - \Delta_2\Delta_3 - \Delta_3\Delta_1} \le 1\,,$$
$$0 \le \Delta_1 + \Delta_2 - \Delta_3,\ 0 \le \Delta_2 + \Delta_3 - \Delta_1,\ 0 \le \Delta_3 + \Delta_1 - \Delta_2\,.$$

Considering the equality in the first expression of the set and having performed identity substitutions, we find that

$$3\left(\Delta_1^2 + \Delta_2^2 + \Delta_3^2\right) - 6\left(\Delta_1\Delta_2 + \Delta_2\Delta_3 + \Delta_3\Delta_1\right) + 2\left(\Delta_1 + \Delta_2 + \Delta_3\right) - 1 = 0\,.$$

This equation determines a conical surface, and the desired region is found by plotting the lines of intersection of this surface with the planes defined with the three last inequalities in the set. The coordinates of the cone apex are $\Delta_1 = \Delta_2 = \Delta_3 = \frac{1}{3}$ coordinates of the intersection of the conical surface with the axes are $\left(\frac{2}{3},0,0\right)$, $\left(0,\frac{2}{3},0\right)$, $\left(0,0,\frac{2}{3}\right)$. The vertex angle of the conical surface apex is $\alpha = \arccos\frac{1}{3}$.

Due to symmetry, the surface bounding the texture parameter variation region can be represented with six elements. The equation for the first part of the conical surface and the first lateral face can be written as

$$r_{cs1}(\nu,\varphi) = r(\varphi)(1-\nu) + r_c\nu\,,\ r_{lf1}(\nu,\varphi) = r(\varphi)\nu\,,\ 0 \le \nu \le 1\,,\ -\frac{\pi}{3} \le \varphi \le \frac{\pi}{3}\,,$$

where $r(\varphi)$ is the equation for the line of intersection of the plane with the conical surface, and r_c is the cone apex.

The remaining parts of the conical surface and the lateral faces bounding the region of texture parameter variation are obtained by rotation of the found elements by the angles $2\pi/3$ and $4\pi/3$ around the axis sloped equally towards the coordinate axes.

The numerically obtained cloud of textured states and the analytically constructed variation region have geometric centers coinciding at the point corresponding to the non-textured state. Both regions possess the required symmetry.

TEXTURE STATE TRAJECTORIES

Various thermal and mechanical treatments are known to lead to variations in the metallic material texture to be manifested in the variations of the corresponding texture parameters. These variations allow a texture state trajectory to be constructed in the general case. As this is being done, each point in the trajectory is matched by certain anisotropy of elastic and plastic properties. Within the framework of solving the problem of attaining efficient plastic anisotropy in metals, Grechnikov et al. in [5] investigated crystallographic texture transformation in the process of continuous hot rolling of aluminum alloys in a 2800 5-stand rolling mill; the corresponding texture parameters were calculated. The evolution of textured states during rolling of an aluminum alloy is represented by varying the positions of the corresponding points in the determined region of texture parameter variation (Fig. 2). All the points are seen to be found within the determined variation region.

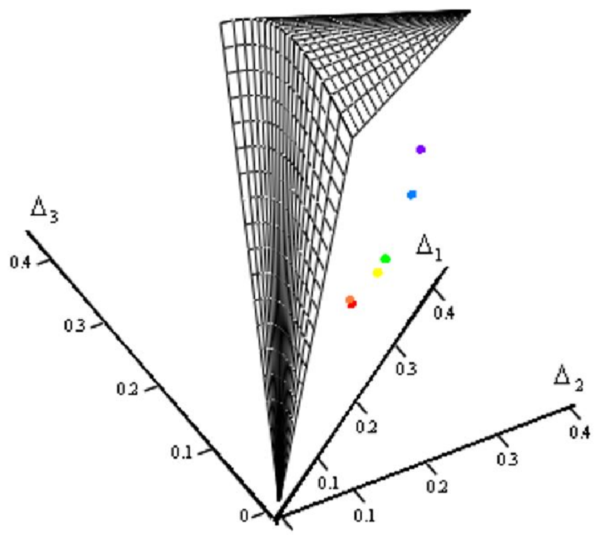


FIGURE 2. The region of texture parameter variation obtained analytically and the textured states of an aluminum alloy after the exit from continuous 2800 roll mill stands: • – initial roll, • – stand 1, • – stand 2, • – stand 3, • – stand 4, • – stand 5

If we introduce a vector $\mathbf{\Delta} = \{\Delta_1, \Delta_2, \Delta_3\}$, then, using the original representation of the Heaviside step function [6] over a segment $t \in [0, T]$, by the values of the texture parameters $\mathbf{\Delta}^{(k)} = \mathbf{\Delta}^{(k)}(t_k)$ in the nodes t_k of the mesh $\Delta_5 \in \{t_0{=}0 < t_1 \ldots t_5 = T\}$, a texture state trajectory can be constructed. Its form is determined by the function $\mathbf{\Delta}(t)$ as

$$\mathbf{\Delta}(t) = \frac{1}{2}\sum_{k=0}^{5}\left[1 + \frac{t-t_k}{(t-t_k)^2} \cdot \frac{t_{k+1}-t}{(t_{k+1}-t)^2}\right]\left\{\mathbf{\Delta}^{(k)}\left(1 - \frac{t-t_k}{t_{k+1}-t_k}\right) + \mathbf{\Delta}^{(k+1)}\frac{t-t_k}{t_{k+1}-t_k}\right\}$$

in the case of linear interpolation.

CONCLUSION

Using analytical and numerical methods for textured cubic polycrystalline materials, the variation region boundaries have been defined for texture parameters, which are regarded integral characteristics of texture to be determined using direct or indirect texture analysis methods. It has been demonstrated that, at various stages of thermal and mechanical treatment of metallic materials, texture evolution can be represented geometrically as a texture state trajectory. With such a representation, each point of the trajectory is matched by a unique anisotropic state, which can be characterized by the known relations comprising anisotropy constants for relevant physical and mechanical properties and texture parameters. The proposed approach can be applied to solving problems of attaining targeted combinations of technological or structural properties of semiproducts and products made of *bcc*- or *fcc*-structured metallic materials.

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